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Summary

Historical perspective on: "Semiclassical trajectory approach to photoisomerisation" by A Warshel and M. Karplus [Chem. Phys. Lett. 32 (1) (1975) 11–17]

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The 2013 Nobel Prize in Chemistry was announced just as this Volume was going to press. It was awarded jointly to Martin Karplus, Michael Levitt and Arieh Warshel '*for the development of multiscale models for complex chemical systems*'.

Martin Karplus and Arieh Warshel have, respectively, published as many as 23 and 13 papers, and two jointly, in *Chemical Physics Letters*. Most of these papers relate to the area of research cited by the Nobel Committee. The Editors of the journal feel it important and timely to include a joint paper from these two Nobelists in this Special Issue. This is particularly appropriate as the citation for their Nobel Prize is central to the field of the journal.

We have chosen a joint work which started to set the theme for the many papers that followed from these authors and others on combining the methods of classical and quantum mechanics to treat complex molecular systems. A semiclassical trajectory scheme is described and applied to the cis–trans isomerisation in the triplet state of butene-2. This is a small system when compared to the biomolecular systems these authors subsequently studied using mixed classical and quantum methods. However, the principles are made clear and allowed for many more extensive applications on the photoisomerisation of more complex molecules as enhanced computing power made this possible in subsequent years.

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